Formal derivation of an exact series expansion for the Principal Field Emission Elliptic Function v

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Abstract

An exact series expansion is now known for the Principal Field Emission Elliptic Function v, in terms of a complementary elliptic variable l' equal to y^2 , where y is the Nordheim parameter. This expansion was originally found by using the algebraic manipulation package MAPLE. This paper presents a formal mathematical derivation. Recently, it has been discovered that v(l') is a particular solution of the ordinary differential equation (ODE) $l'(1-l')d^2v/dl'^2 = nv$, when the index n = 3/16. This ODE appears to be new in mathematical physics and ellipticfunction theory. The paper first uses an 1876 result from Cayley to establish the boundary condition that dv/dl' satisfies as l' tends to zero. It then uses the method of Frobenius to obtain two linearly independent series solutions for the ODE, and hence derives the series expansion for v(l'). It is shown that terms in $\ln l'$ are required in a mathematically correct solution, but fractional powers of l' are not. The form of the ODE also implies that simple Taylor expansion methods cannot generate good approximation formulae valid over the whole range $0 \le l' \le 1$; this conclusion may also apply to barriers of other shapes. It is hoped that this derivation might serve as a paradigm for the treatment of other tunnelling barrier models for cold field electron emission, if in any particular case an ODE can be found for which the tunnelling-exponent correction function is a particular solution.

1 Introduction

Fowler-Nordheim (FN) tunnelling [1] is electric-field-induced electron tunnelling through a roughly triangular barrier. When the emission barrier is strong and the penetration coefficient small, there is a low-temperature emission regime (including room temperature) known as "cold field electron emission (CFE)". Tunnelling and CFE are processes of significant technological interest, in particular for the prevention of vacuum breakdown, the development of cold-cathode electron sources, and internal electron transfer processes in some types of electronic device. Tunnelling and CFE are at the heart of several multi-billion-dollar industries.

CFE from a metal-like conduction band is described by a family of approximate equations known as "Fowler-Nordheim-type" (FN-type) equations. FN-type equations for the emission-current density J, as a function of the local work-function ϕ and the local barrier field F, have the form

$$J = \lambda a \phi^{-1} F^2 \exp(-\mu b \phi^{3/2} / F) \tag{1}$$

where a and b are the First and Second FN Constants as usually defined (e.g. [2]), and λ and μ are generalised correction factors. The forms of λ and μ depend on the assumptions and

approximations made in the derivation, in particular on the shape assumed for the tunnelling barrier.

For a planar emitter, a "Schottky-Nordheim" (image-rounded) barrier model [3, 4] is normally used. In this case, μ is given by the mathematical parameter $v_{\rm F}$, which is a particular value (see below) of the Principal Field Emission Elliptic Function v. This function v is obtained by applying the simple-JWKB approximation [5, 6] to a Schottky-Nordheim (SN) barrier, and can be defined by a JWKB integral (see, for example, [7]). Although always called an "elliptic function", v is better described as a special kind of complete elliptic integral. An expression for v in terms of the complete elliptic integrals of the first and second kinds, K(m) and E(m), where m is the elliptic parameter as used in [8], has been known for many years, and numerical values have long been available [9].

Recently, [7, 10], an exact series expansion (see below) has been found for v, in terms of the elliptic variable l' defined by

$$l' = [(1-m)/(1+m)]^2. (2)$$

It follows that

$$m(l') = (1 - \sqrt{l'})/(1 + \sqrt{l'}).$$
 (3)

The primed symbol l' was chosen, in accordance with a normal convention in elliptic-function theory, because l' is a "complementary" elliptic variable in the sense that $l' \to 0$ as $m \to 1$. Knowing the form of the exact expansion for v(l') has enabled us to develop [7] numerical approximation formulae for v(l') and dv/dl', with absolute error $|\epsilon| < 7 \times 10^{-10}$, that substantially outperform earlier numerical approximations of equivalent complexity [11]. It also provides a mathematical explanation for the success of the simple approximation formula [7, 10]

$$v(l') \approx 1 - l' + (1/6) l' \ln l',$$
 (4)

which has the merits that it is exact at l'=0 and l'=1, and (when assessed over the whole range $0 \le l' \le 1$) has absolute error $|\epsilon| < 0.0025$ and outperforms all existing formulae of equivalent complexity [7].

In CFE, the physical parameter f (the "scaled barrier field") is defined by $f = F/F_{\phi}$, where F_{ϕ} is the barrier field necessary to reduce to zero a barrier of zero-field height ϕ . The values of F and f determine the strength of the tunnelling barrier. For the SN barrier, this physical parameter f can be identified with the mathematical parameter l', and μ in eq. (1) is given by v(l' = f).

The complete elliptic integrals of the first and second kinds may be defined [8] in terms of the elliptic parameter m by

$$K(m) = \int_0^{\pi/2} \frac{d\phi}{\sqrt{1 - m\sin^2\phi}}$$
 and $E(m) = \int_0^{\pi/2} \sqrt{1 - m\sin^2\phi} \,d\phi.$ (5)

Using (3), K and E can, in principle, be expressed in terms of l' rather than m. The expression for v(l') in terms of K and E then is [7]:

$$v(l') = (1 + \sqrt{l'})^{1/2} \left[E(m(l')) - \sqrt{l'} K(m(l')) \right]$$
(6)

where m(l') is given by equation (3).

The exact series expansion for v(l') was originally generated [10] by the algebraic manipulation package MAPLE, by expanding an expression equivalent to (6). Numerical values obtained from MAPLE agreed with values obtained by numerical evaluation of the relevant JWKB integral, to better than 12 decimal places, strongly indicating that both methods were mathematically sound. We subsequently found algebraic formulae that reproduced the MAPLE result (see [7], Appendix 1). However, "manual" derivation of higher-order terms in v(l') is excessively laborious; also, this method does not bring out the underlying mathematics.

Seeking a better mathematical derivation, we found [7] that v(l') is a particular solution of the ordinary differential equation (ODE)

$$l'(1-l')\frac{d^2W}{dl'^2} = nW, (7)$$

when n=3/16 and certain boundary conditions (see below) are satisfied. Equation (7) appears to be new to mathematical physics and elliptic-function theory. Its solution has not been found in easily available mathematical literature, but does not involve any new mathematical principles. Applying the method of Frobenius [12] generates a series expansion with coefficients defined by recurrence relations (see below). These formulae correctly generate the numerical coefficients already reported [10].

This finding has itself been reported [7], but the full proof was too lengthy to include in earlier work. This paper presents the full mathematical derivation of the relevant recurrence relations. In part, the aim is to provide closure on the mathematics of the (simple-JWKB treatment of the) SN barrier; but we hope this method might also be a paradigm for finding exact solutions for correction factors for barriers of other shapes. It would be applicable where a method can be found for converting the JWKB-type integral definition of the correction function into an equivalent differential equation.

The structure of the paper is as follows. Section 2 derives boundary conditions that v must satisfy, Section 3 derives general solutions for (7), Section 4 uses these to derive a series expansion for v, and Section 5 provides discussion.

2 Boundary conditions

To establish the expansion for v, we need the boundary conditions that v(l') and dv/dl' satisfy at l' = 0. It is well known in CFE theory that v(0) = 1. However, dv/dl' becomes infinite as $l' \to 0$, so the boundary condition on dv/dl' has to take the slightly unusual form that "dv/dl' becomes infinite in the correct way". We develop both conditions from a result proved by Cayley in his 1876 textbook [14]. This section is presented in the form of three lemmas.

Lemma 1 As l' approaches zero from above, the function K(m(l')) is given by

$$K(m(l')) = (3/2) \ln 2 - (1/4) \ln l' + O(\sqrt{l'}). \tag{8}$$

Proof. From (3), we have

$$(1-m) = \frac{2\sqrt{l'}}{1+\sqrt{l'}}.$$

Formula 17.3.26 in [8] is derived from Cayley's result and states that

$$\lim_{m \to 1} K(m) = \ln \left[4/\sqrt{(1-m)} \right].$$

Hence

$$\lim_{l' \to 0} K(m(l')) = \lim_{l' \to 0} \ln \left[4\sqrt{\frac{1 + \sqrt{l'}}{2\sqrt{l'}}} \right] = \lim_{l' \to 0} \left[(3/2) \ln 2 - (1/4) \ln l' + O(\sqrt{l'}) \right],$$

as required. We have thus proved a Cayley-type result for K as a function of l'. This result is key to deriving the series expansion for v.

Lemma 2 v(0) = 1.

Proof. Using lemma 1, we find that, in the limit of small l', the term involving K(m(l')) in definition (6) takes the form

$$-\lim_{l'\to 0} \left[(1+\sqrt{l'})^{1/2} \sqrt{l'} [(3/2) \ln 2 - (1/4) \ln l'] \right] = 0.$$

When l'=0, then m=1, and the term in E(m(l')) in definition (6) reduces to

$$E(m=1) = \int_0^{\pi/2} \cos \phi \, d\phi = 1.$$

It follows that v(0) = 1. This is a well-known result in CFE theory, but for completeness we have given formal proof here.

Lemma 3

$$\lim_{l' \to 0} \left[\frac{\mathrm{d}v}{\mathrm{d}l'} - (3/16) \ln l' \right] = -(9/8) \ln 2 \tag{9}$$

Proof. From [7] we have the result that

$$\frac{\mathrm{d}v}{\mathrm{d}l'} = -\frac{3K(m(l'))}{4\left(1+\sqrt{l'}\right)^{1/2}}.$$
(10)

Using (8), we have, for small l', that

$$\frac{\mathrm{d}v}{\mathrm{d}l'} \approx -\frac{3}{4} \left[1 - \frac{\sqrt{l'}}{2} \right] \left[\frac{3}{2} \ln 2 - \frac{1}{4} \ln l' \right].$$

The limiting form for dv/dl' in (9) follows.

3 General solution of the ODE

We now solve the ODE. Mathematically, it is convenient to solve the general equation, i.e. (7), and then put n equal to 3/16. We use the symbol W to denote a general solution of the relevant equation, whether the index is taken generally as n or specifically as 3/16.

We use the method of Frobenius [12, 13] to find a series expansion for W(l'). Initially assume a power series solution of the form $l'^r \sum_{i=0}^{\infty} g_i l'^i$, where r and the g_i are to be determined. Substituting into (7) and equating powers of l', we find

$$g_0 r(r-1)l'^{r-1} + l'^r \sum_{i=0}^{\infty} l'^i [-(i+r-1)(i+r)g_i - ng_i + (i+r)(i+r+1)g_{i+1}] = 0.$$
 (11)

Since this is an identity for all powers of l', the first term has to be identically zero and there is a recurrence relation for the coefficient g_i :

$$g_{i+1} = \frac{(i+r-1)(i+r)+n}{(i+r)(i+r+1)}g_i, \quad i \ge 0.$$
 (12)

Obviously, if $g_0 = 0$ then all g_i ($i \ge 1$) are also zero, and W is identically equal to 0; so the $g_0 = 0$ case cannot contribute to the general solution. Hence, we deduce that the indicial equation is r(r-1) = 0. This equation has the two roots $r_1 = 1, r_2 = 0$. Since $|r_1 - r_2|$ is an integer, two linearly independent solutions W_A, W_C are [12, 13]:

$$W_{\mathcal{A}}(l') = \alpha W_1(l'),\tag{13}$$

$$W_{\rm C}(l') = \chi [W_2(l') + W_1(l') \ln l'], \tag{14}$$

where α and χ are arbitrary constants. We take α equal to unity, without loss of generality, but leave χ to be chosen appropriately later. $W_1(l')$ and $W_2(l')$ are the series expansions that correspond to the values r = 1, r = 0, respectively, and are written in the forms

$$W_1(l') = l' \sum_{i=0}^{\infty} a_i l'^i, \quad W_2(l') = \sum_{i=0}^{\infty} b_i l'^i,$$
 (15)

where the a_i and b_i are coefficients to be determined. The general solution of (7) can thus be put in the form

$$W(l') = AW_{\mathcal{A}}(l') + CW_{\mathcal{C}}(l') \tag{16}$$

where A and C are arbitrary constants to be determined by the boundary conditions, and the two independent solutions have the forms

$$W_{\rm A}(l') = \sum_{i=0}^{\infty} a_i l'^{i+1}.$$
 (17)

$$W_{\rm C}(l') = \chi \left[\sum_{i=0}^{\infty} b_i l'^i + l' \ln l' \sum_{i=0}^{\infty} a_i l'^i \right].$$
 (18)

Note that the multiplier $l' \ln l'$ is an intrinsic part of the correct mathematical solution of (7). The coefficients a_i have the properties of the coefficients g_i when r is taken as 1 in (11). So, from (12):

$$a_{i+1} = \frac{i(i+1)+n}{(i+1)(i+2)} a_i, \quad i \ge 0.$$
(19)

As far as the solution W_A is concerned, the value of a_0 can be chosen arbitrarily without loss of generality, because all values of a_i ($i \ge 1$) are proportional to a_0 .

To determine the coefficients b_i , we substitute form (18) into (7), eliminate the terms in $\ln l'$ by noting that W_1 is a solution [hence, $l'(1-l')d^2W_1/d l'^2 - nW_1 = 0$], expand $W_2(l')$ in series form, and eventually obtain

$$n(b_0 + b_1 l') - 2b_2 l' + \sum_{i=0}^{\infty} \left(\left[\left\{ (i+1)(i+2) + n \right\} b_{i+2} - (i+2)(i+3)b_{i+3} \right] l'^{i+2} \right) + \sum_{i=0}^{\infty} c_i l'^i = 0.$$
 (20)

where

$$\sum_{i=0}^{\infty} c_i l'^i = 2(l'-1) dW_1/dl' - (1-1/l')W_1 = (l'-1) \sum_{i=0}^{\infty} (2i+1) a_i l'^i.$$
 (21)

Hence

$$c_0 = -a_0$$
 and $c_i = (2i-1)a_{i-1} - (2i+1)a_i, i \ge 1.$ (22)

In order for (20) to be an identity, we need the coefficients of l'^0 and l'^1 to be zero, which requires that: $c_0 + nb_0 = 0$; and $c_1 + nb_1 - 2b_2 = 0$. This yields

$$b_0 = -c_0/n = a_0/n, (23)$$

$$b_2 = (c_1 + nb_1)/2 = (a_0 - 3a_1 + nb_1)/2.$$
(24)

More generally, the requirement that in (20) the coefficient of l^{i} be zero yields

$$\{(i+1)(i+2)+n\}b_{i+2}-(i+2)(i+3)b_{i+3}+c_{i+2}=0, i\geq 0,$$
(25)

which on re-arrangement yields

$$b_{i+1} = \frac{c_i + \{(i-1)i + n\}b_i}{i(i+1)}, \quad i \ge 2.$$
(26)

Equation (26) also gives b_2 correctly; so, using (22), we can write

$$b_{i+1} = \frac{(2i-1)a_{i-1} - (2i+1)a_i + \{(i-1)i + n\}b_i}{i(i+1)}, \quad i \ge 1.$$
(27)

In summary, the value of b_0 is fixed by (23), and the values of b_i ($i \ge 2$) are determined, via (27), by the choice of b_1 .

If $W_{\rm C}$ is to be a linearly independent solution of (7), then any multiple of $W_{\rm C}$ must also be a solution. We can satisfy this requirement by ensuring that each of the coefficients a_i, b_i is individually proportional to a_0 . This is already true for all the a_i and for b_0 . It is sufficient that we further put

$$b_1 = \beta a_0, \tag{28}$$

where β is a constant to be chosen; from (27), this ensures that all b_i ($i \geq 2$) are proportional to a_0 .

At this point, we have derived general forms for two linearly independent solutions of (7). To derive specific forms for these independent solutions, we need to choose values for a_0 , β and χ . In principle, these might be chosen in various ways. We choose them here in such a way as to make the boundary conditions at l' = 0 straightforward to apply.

From equations (16) to (18), and (23), the form for W(l'), up to terms involving l', is:

$$W(l') = Ca_0\chi/n + (Aa_0 + C\chi\beta a_0)l' + C\chi a_0l' \ln l' + \dots,$$
(29)

and the corresponding form for dW/dl' is

$$dW/dl' = Aa_0 + C\beta \chi a_0 + C\chi a_0 + C\chi a_0 \ln l' + \dots$$
(30)

From (29), when l' = 0:

$$C = (n/\chi)(W_0/a_0). (31)$$

where $W_0=W(0)$. Clearly, a convenient way to deal with (30) is to choose $\beta=-1$. Equations (29) and (30) are now reduced to

$$W(l') = W_0 + [Aa_0 - nW_0]l' + nW_0l' \ln l' + \dots$$
(32)

$$dW/dl' = Aa_0 + nW_0 \ln l' + \dots$$
(33)

Since these equations contain a_0 only in the combination Aa_0 , we can take $a_0 = 1$ without loss of generality; then $b_0 = 1/n$ and $b_1 = -1$. Values of a_i $(i \ge 1)$ and b_i $(i \ge 2)$ can then be obtained from the recurrence formulae above.

At this point, we have the situation that $W_A(0) = 0$ and

$$W_{\rm C}(0) = \chi b_0 = \chi/n \tag{34}$$

It is convenient to have $W_{\rm C}(0) = 1$, so we choose $\chi = n$, which also simplifies (31) to

$$C = W(0)/a_0 = W(0). (35)$$

This completes the definition of two convenient, linearly independent solutions of ODE (7), and enables the general solution to be written in the form

$$W(l') = 1 + \sum_{i=0}^{\infty} (Aa_i + Cnb_{i+1} + Cna_i \ln l')l'^{i+1},$$
(36)

where $a_0 = 1, b_1 = -1$, and the other coefficients are given by the recurrence relations (19) and (25). Note that this form (and the value derived below for C) differ slightly from a form proposed earlier [15], because we have defined $W_{\rm C}$ in a slightly different (more convenient) way here.

4 Series expansion for function v

At this point, we revert to discussion of the ODE of index 3/16, and derive the expansion for v(l'). For n = 3/16, the first few terms of the two independent solutions are

$$W_{\rm A}(l') = l' + \frac{3}{32}l'^2 + \frac{35}{1024}l'^3 + \dots,$$
 (37)

$$W_{\rm C}(l') = 1 - \frac{3}{16}l' + \frac{51}{1024}l'^2 + \frac{177}{8192}l'^3 + \dots + \left(\frac{3}{16} + \frac{9}{512}l' + \frac{105}{16384}l'^2 + \dots\right)l'\ln l'. \tag{38}$$

Using the boundary condition $W_0 = v(0) = 1$, (35) yields C = 1. For the second boundary condition we use (as noted earlier) the slightly unusual requirement that, as l' tends to zero, the derivative dW/dl' "tends to infinity in the correct way". Comparing (9) and (33) yields the following identity, valid in the limit of small l'-values:

$$(3/16) \ln l' - (9/8) \ln 2 = nW_0 \ln l' + Aa_0 \tag{39}$$

Since n = 3/16 and $W_0 = 1$, the terms in $\ln l'$ cancel. So, since $a_0 = 1$:

$$A = -(9/8)\ln 2. \tag{40}$$

So the first few terms of the expansion for v(l') are:

$$v(l') = 1 - \left(\frac{9}{8}\ln 2 + \frac{3}{16}\right)l' - \left(\frac{27}{256}\ln 2 - \frac{51}{1024}\right)l'^2 - \left(\frac{315}{8192}\ln 2 - \frac{177}{8192}\right)l'^3 + \dots + l'\ln l'\left(\frac{3}{16} + \frac{9}{512}l' + \frac{105}{16384}l'^2 + \dots\right).$$

$$(41)$$

This series has the form reported earlier [7, 10], found by using MAPLE. Evaluating the coefficients to 5 decimal places yields

$$v(l') = 1 - 0.96729l' - 0.02330l'^2 - 0.00505l'^3 + \dots + l' \ln l' (0.18750 + 0.01758l' + 0.00641l'^2 + \dots). \tag{42}$$

By dividing the first expression by 1 - l', this can be put into a form that is exact at both l' = 0 and l' = 1, even when the two series expansions below are truncated:

$$v(l') = (1 - l')(1 + 0.03271l' + 0.00941l'^{2} + \dots) + l' \ln l'(0.18750 + 0.01758l' + 0.00641l'^{2} + \dots).$$
(43)

Both of the series in (43) have good convergence properties in the range $0 \le l' \le 1$, so this form is useful for numerical approximations [7].

5 Discussion

For most of the last 50 years, the correction function v has been expressed in CFE theory as a function of the Nordheim parameter $y = \sqrt{l'}$ [4], rather than l'. In [10] it was argued that, because the exact series expansion (41) contains no terms in $\sqrt{l'}$, it is mathematically more natural to use l' as the independent variable. The derivation here, using the method of Frobenius, confirms this formally. Terms in $\ln l'$ are an intrinsic part of the correct mathematical solution, but fractional powers of l' are not necessary.

Approximate formulae such as (4) cannot be derived by simple Taylor expansion methods. It is implicit in the mathematical analysis here that simple Taylor expansion methods cannot generate good approximate formulae valid for the whole range $0 \le l' \le 1$. This conclusion may also be applicable to tunnelling barriers of other shapes.

Equation (7), the defining ODE, can be transformed to be in terms of the variable y. This yields

$$(1-y^2)\frac{d^2W}{dy^2} + \frac{1-y^2}{y}\frac{dW}{dy} - \frac{3}{4}W = 0.$$
(44)

Obviously, this equation is more complex than (7). This is a further good mathematical reason for choosing to use the variable l', rather than y, in CFE theory. As discussed elsewhere [7], an important implication of the role of l' in the mathematics is that the natural variable to use in physical discussions of CFE theory is the scaled barrier field f.

The algebraic manipulation package MAPLE has played a crucial role in stimulating this work, because our use of MAPLE [10] drew attention to the existence and form of the series expansion for v(l') and provided a result to aim for. Derivation of this series by inserting series expansions for K(l') and E(l') into (6) proved excessively laborious if performed by hand [7], even when we had found the Cayley forms [14] for the series expansions of K(m) and E(m), (which, interestingly, are not reported in several of the elliptic-function handbooks consulted). So we looked for the ODE that v(l') obeyed and found (7) [7].

Luckily, the ODE (7) has a very simple form. Nevertheless, the derivation of solutions is quite a lengthy mathematical process. Wylie [12] (p. 322) describes the solution of equations of this general kind as "straightforward but very tedious"; we confirm his description. Much of Section 3 here could, in principle, have been written in the late 1800s, or at any subsequent time, but there has been little incentive to do so.

Overall, it is not entirely surprising that getting a series expansion/definition for v in place has taken nearly 80 years, measured from the original (incorrect) attempt by Nordheim [4] to derive an exponent correction function for the SN barrier. Essentially, it is the relatively recent introduction of reliable computer algebra packages that has made the discovery of this expansion (and its mathematical origin) feasible, rather than so difficult as to be unlikely to happen. The problem for CFE and the SN barrier (even when using the simple-JWKB approximation) has been that the necessary mathematical functions have not been solidly in place when physicists needed them, in the 1920s and 1950s; one might contrast this with the wave-mechanical analysis of the hydrogen atom in the 1910s, which needed mathematical functions that had been well defined for very many years.

As indicated in the introduction, our hope is that the derivation in this paper may be able to serve as a paradigm for the treatment of other barrier models, particularly for realistic models for the potential-energy variation above sharply curved emitters. The keys, in each case, will be to find an ODE that the tunnelling-exponent correction function satisfies, and a suitable formulation of the boundary conditions.

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